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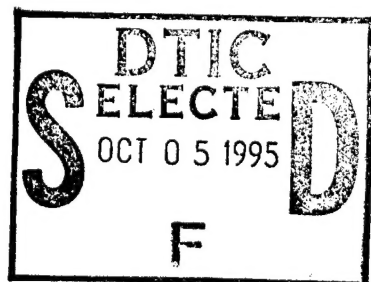
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# WORKSHOP ON NEW OPTIMIZATION TECHNIQUES FOR LARGE COMPOUNDS

FINAL REPORT FOR AFOSR GRANT F49620-93-1-0112

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DEPARTMENT OF CHEMISTRY  
IOWA STATE UNIVERSITY

## ABSTRACT

The purpose of this grant was to support a workshop devoted to the development, testing and applications of "New Optimization Methods for Global and Local Structural Optimization". This topic was the subject of a new AFOSR initiative begun in FY'94. The workshop was held at Iowa State University, in Ames, Iowa, on January 15-16, 1993, with participation of approximately 20 experts in the field (chemists, mathematicians, computer scientists, chemical engineers and biochemists) who expressed an interest in participating in the initiative, several representatives of AFOSR, and several scientists from Air Force Laboratories. A number of Iowa State University scientists attended as well. The workshop was an intensive two days of scientific sessions, in which the best approaches to optimization problems were explored. The role of parallel computing in addressing these problems was also discussed. An important consequence of this workshop was a successful initiative competition in the area of global optimization. Nearly all of the successful proposals were submitted by workshop participants.

On May 1-2, 1995, a follow-up workshop on the same subject was held in Washington, DC, at the Georgetown National Academy of Sciences Building. Participants included cognizant representatives from AFOSR and Air Force Laboratories, all scientists who submitted successful proposals to the global optimization initiative, scientists funded in other AFOSR programs, and the original workshop PI. This was a highly successful exchange of ideas that clearly raised important issues in the area. The most exciting aspect of both workshops was the development of collaborations among scientists in areas of science (e.g., chemistry, computer science, mathematics biochemistry) who often are not even aware of each others' research.

## OBJECTIVES

Many problems of importance to the Air Force involve intimate knowledge of the properties and reactivity of species which contain large numbers (from 20 to thousands)

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of atoms. Examples of such systems are: (a) species which are potential new high energy fuels, such as metals with low mass embedded in solid hydrogen; (b) new nonlinear optical (NLO) polymers currently under investigation in the Wright Laboratories and by several contractors; (c) new lubricants; and (d) a variety of composite materials. Theoretical investigations are expected to play a major role in developing an understanding of such species, thereby making the development of new materials more efficient and cost-effective.

A central problem in the application of theoretical chemical methods to systems of many atoms is the determination of the stationary points (minima, transition states) on the potential energy surface. While very effective optimization methods have been developed for molecules with small numbers of atoms, these methods have limited usefulness for systems of prime interest to the Air Force. Some methods have been developed to study new drug compounds and other species of biological importance, but these methods have proved to be largely ineffective, and the potentials used in that area of research are mostly too oversimplified for our purposes.

There is therefore a critical need to develop new effective and computationally efficient methods for global and local optimizations of large species. The **specific objectives** of the proposed workshop were to:

1. Educate the optimization community regarding the specific needs of the Air Force.
2. Promote discussions among the participating scientists regarding potential solutions of the central problem.
3. Facilitate interactions among theoretical chemists, mathematicians, computer scientists, and Air Force laboratory scientists, in order to develop the broadest possible approach to addressing optimization problems.
4. Consider the role supercomputing in general and parallel computing in particular can play in solving these problems.

#### **JANUARY WORKSHOP**

The participants in the January 1993 workshop at Iowa State University were:

## UNIVERSITY PARTICIPANTS

C. Bajaj, Computer Science, Purdue University  
R. Byrd, Computer Science, University of Colorado  
J. Caruthers, Engineering, Purdue University  
A. DePristo, Chemistry, Iowa State University  
S. Elbert, Chemistry, Iowa State University  
D. Ferguson, Medicinal Chemistry, University of Minnesota  
C. Floudas, Chemical Engineering, Princeton University  
M. Gordon, Chemistry, Iowa State University  
T. Holme, Chemistry, University of South Dakota  
A. Komornicki, Polyatomics Research Institute  
L. Lasdon, Management Science, University of Texas  
T. Magee, Business, University of Colorado-Boulder  
T. Morin, Engineering, Purdue University  
J. Pekny, Chemical Engineering, Purdue University  
P. Pulay, Chemistry, University of Arkansas  
H. Rabitz, Chemistry, Princeton University  
S. Robinson, Industrial Engineering, University of Wisconsin  
B. Rosen, Computer Science, University of Minnesota  
B. Schlegel, Chemistry, Wayne State University  
B. Schnabel, Computer Science, University of Colorado-Boulder  
S. Schwartz, Albert Einstein College of Medicine  
D. Shalloway, Biotechnology, Cornell University  
J. Simons, Chemistry, University of Utah  
P. Taylor, Chemistry, San Diego Supercomputer Center  
D. Thirumalai, Chemistry, University of Maryland  
J. Weare, Chemistry, University of California-San Diego

## **AFOSR PARTICIPANTS**

L. Burggraf, AFOSR/NC  
T. Erstfeld, AFOSR/NC  
N. Glassman, AFOSR/NM

## **PARTICIPANTS FROM AIR FORCE LABORATORIES**

J. Boatz, Phillips Laboratory (AL)  
M. Coolidge, Seiler Laboratory  
L. Merkle, AFIT-Wright-Patterson  
R. Pachter, Wright Laboratories  
S. Rodgers, Phillips Laboratory (AL)

The following is the schedule of presentations at the January workshop:

### SCHEDULE OF EVENTS

Friday, January 15, 1993

Spedding Hall, Room 301B, ISU Campus

Coffee, juice and rolls provided

08:30 Introductory remarks

Neal Glassman

Mark Gordon

Session 1, Ruth Pachter (WL), presiding

09:00 - 09:30 John Weare (University of California - San Diego)

09:30 - 10:00 Bobby Schnabel (University of Colorado - Boulder)

10:00 - 10:30 Tim Magee (University of Colorado - Boulder)

10:30 - 11:00 break

Session 2, Jerry Boatz (PL), presiding

11:00 - 11:30 Herschel Rabitz (Princeton University)

11:30 - 12:00 Chris Floudas (Princeton University)

12:00 - 12:30 David Thirumalai (University of Maryland)

12:30 - 14:00 lunch

Session 3, Larry Burggraf (AFOSR), presiding

14:00 - 14:30 Steven Schwartz (Albert Einstein College of Medicine)

14:30 - 15:00 David Shalloway (Cornell University)

15:00 - 15:30 Andy Komornicki (Polyatomics Research Institute)

15:30 - 16:00 break

16:00 - 16:30 Berny Schlegel (Wayne State University)

16:30 - 17:30 round table discussion

Saturday, January 16

Gateway Holiday Inn

Coffee, juice, and rolls provided

Session 4, Mark Gordon (Iowa State University), presiding

08:30 - 09:00 Ben Rosen (University of California - San Diego)

09:00 - 09:30 Steve Robinson (University of Wisconsin)

09:30 - 10:00 Chanderjit Bajaj (Purdue University)

10:00 - 10:30 break

Session 5, Neal Glassman (AFOSR), presiding

10:30 - 11:00 Leon Lasdon (University of Texas)

11:00 - 11:30 Tom Morin (Purdue University)

11:30 - 12:30 Round Table Discussion

12:30 - 2:00 lunch

Session 6, Mike Coolidge (Air Force Academy), presiding

14:00 - 14:30 Peter Taylor (San Diego Supercomputer Center)

14:30 - 15:00 Jack Simons (University of Utah)

15:00 - 15:30 Peter Pulay (University of Arkansas)

15:30 - 16:00 break

16:00 - 17:00 round table discussion

17:00 closing remarks

## **OUTCOMES OF JANUARY WORKSHOP**

The January workshop had several positive outcomes:

- Exchange of ideas among scientists from several areas of science and engineering.
- Exposure of Air Force personnel to the current state-of-the-art in optimization methods.
- Heightening of awareness in the community of the importance of scalable computing for solving large problems.
- Development of inter-disciplinary collaborations (Schnabel-Weare, Schnabel-Schlegel)
- Focused goals of the subsequent RFP for the Initiative on Optimization

## **FOLLOW-UP WORKSHOP**

The participants at the follow-up workshop held in Washington, DC, in May 1995 were:

Professor Alexander, University of Maryland  
Professor Bajaj, University of Minnesota  
Dr. Berman, AFOSR  
Dr. Boatz, Air Force Phillips Laboratory  
Dr. Glassman, AFOSR  
Professor Gordon, Iowa State University  
Professor Floudas, Princeton University  
Dr. Head-Gordon, LBL  
Dr. Pachter, Wright Laboratories  
Professor Pulay, University of Arkansas  
Professor Rabitz, Princeton University  
Dr. Rodgers, Air Force Phillips Laboratory  
Professor Shalloway, Cornell University  
Dr. Schmidt, Iowa State University  
Professor Schnabel, University of Colorado  
Professor Thirumalai, University of Maryland  
Professor Weare, University of California-San Diego  
Dr. Yeates, Wright Laboratories

The schedule for the follow-up workshop was:

Ida and Cecil Green Building  
Room Green 120  
2001 Wisconsin Avenue  
Washington DC 20007

Monday, May 1



8:00-8:20	Coffee
8:20-8:30	Opening Remarks (Glassman, Rodgers, Berman)
8:30-9:15	Prof Weare
9:15-10:30	Prof Pulay
10:30-10:45	Break
10:45-11:30	Prof Thirumalai
11:30-12:15	Dr Dudis
12:15-1:45	Lunch
1:45-2:30	Dr Rodgers
2:30-3:15	Prof Bajaj
3:15-3:30	Break
3:30-4:15	Prof Shalloway

#### Tuesday May 2

8:00-8:30	Coffee
8:30-9:15	Dr Pachter
9:15-10:30	Dr Head-Gordon
10:30-10:45	Break
10:45-11:30	Prof Floudas, Prof Rabitz
11:30-12:15	Prof Schnabel

The main purpose of the follow-up workshop was to provide a forum in which the participants in the initiative could present the preliminary results of their research. A secondary purpose was to solidify existing collaborations and to encourage new ones. Based on the enthusiastic discussions, this was a very successful meeting.